## Kulbir K Ghuman

List of Publications by Year in descending order

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KILIBID K CHUMAN

#	Article	IF	CITATIONS
1	Photoexcited Surface Frustrated Lewis Pairs for Heterogeneous Photocatalytic CO <sub>2</sub> Reduction. Journal of the American Chemical Society, 2016, 138, 1206-1214.	13.7	210
2	llluminating CO <sub>2</sub> reduction on frustrated Lewis pair surfaces: investigating the role of surface hydroxides and oxygen vacancies on nanocrystalline In <sub>2</sub> O <sub>3â<sup>°</sup>x</sub> (OH) <sub>y</sub> . Physical Chemistry Chemical Physics, 2015, 17, 14623-14635.	2.8	186
3	Amorphous TiO2 as a Photocatalyst for Hydrogen Production: A DFT Study of Structural and Electronic Properties. Energy Procedia, 2012, 29, 291-299.	1.8	108
4	Adsorption and Dissociation of H <sub>2</sub> O on Monolayered MoS <sub>2</sub> Edges: Energetics and Mechanism from <i>ab Initio</i> Simulations. Journal of Physical Chemistry C, 2015, 119, 6518-6529.	3.1	107
5	Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO <sub>2</sub> with High Activity and Tailored Selectivity. Advanced Science, 2017, 4, 1700252.	11.2	97
6	Heterogeneous reduction of carbon dioxide by hydride-terminated silicon nanocrystals. Nature Communications, 2016, 7, 12553.	12.8	93
7	Tailoring Surface Frustrated Lewis Pairs of In <sub>2</sub> O <sub>3â``</sub> <i><sub>x</sub></i> (OH) <sub>y</sub> for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO <sub>2</sub> by Isomorphous Substitution of In <sup>3+</sup> with Bi <sup>3+</sup> . Advanced Science. 2018. 5. 1700732.	11.2	91
8	Shining light on CO <sub>2</sub> : from materials discovery to photocatalyst, photoreactor and process engineering. Chemical Society Reviews, 2020, 49, 5648-5663.	38.1	91
9	Carrier dynamics and the role of surface defects: Designing a photocatalyst for gas-phase CO <sub>2</sub> reduction. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8011-E8020.	7.1	89
10	Enhanced photothermal reduction of gaseous CO <sub>2</sub> over silicon photonic crystal supported ruthenium at ambient temperature. Energy and Environmental Science, 2018, 11, 3443-3451.	30.8	83
11	Surface Analogues of Molecular Frustrated Lewis Pairs in Heterogeneous CO <sub>2</sub> Hydrogenation Catalysis. ACS Catalysis, 2016, 6, 5764-5770.	11.2	80
12	Metadynamics-Biased ab Initio Molecular Dynamics Study of Heterogeneous CO <sub>2</sub> Reduction via Surface Frustrated Lewis Pairs. ACS Catalysis, 2016, 6, 7109-7117.	11.2	78
13	Highly Efficient Ambient Temperature CO <sub>2</sub> Photomethanation Catalyzed by Nanostructured RuO <sub>2</sub> on Silicon Photonic Crystal Support. Advanced Energy Materials, 2018, 8, 1702277.	19.5	58
14	Effect of doping on electronic structure and photocatalytic behavior of amorphous TiO2. Journal of Physics Condensed Matter, 2013, 25, 475501.	1.8	30
15	Mechanistic insights into water adsorption and dissociation on amorphous TiO <sub>2</sub> -based catalysts. Science and Technology of Advanced Materials, 2018, 19, 44-52.	6.1	25
16	A DFT + <i>U</i> study of (Rh, Nb)-codoped rutile TiO <sub>2</sub> . Journal of Physics Condensed Matter, 2013, 25, 085501.	1.8	23
17	Structure factor of amorphous TiO2 nanoparticle; Molecular Dynamics Study. Journal of Non-Crystalline Solids, 2011, 357, 3399-3404.	3.1	19
18	Self-Trapped Charge Carriers in Defected Amorphous TiO <sub>2</sub> . Journal of Physical Chemistry C, 2016, 120, 27910-27916.	3.1	17

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19	Strained structure of differently prepared amorphous TiO <sub>2</sub> nanoparticle: Molecular dynamics study. Journal of Materials Research, 2011, 26, 2604-2611.	2.6	14
20	Role of surface engineering of hybrid structure for high performance quantum dots based photoelectrochemical hydrogen generation. Chemical Engineering Journal, 2022, 429, 132425.	12.7	14
21	Tailoring widely used ammonia synthesis catalysts for H and N poisoning resistance. Physical Chemistry Chemical Physics, 2019, 21, 5117-5122.	2.8	13
22	Molecular dynamics study of oxygen-ion diffusion in yttria-stabilized zirconia grain boundaries. Journal of Materials Chemistry A, 2022, 10, 2567-2579.	10.3	11
23	Solar Fuels: Highly Efficient Ambient Temperature CO <sub>2</sub> Photomethanation Catalyzed by Nanostructured RuO <sub>2</sub> on Silicon Photonic Crystal Support (Adv. Energy Mater. 9/2018). Advanced Energy Materials, 2018, 8, 1870041.	19.5	7
24	Electronic Structure of a Polybenzimidazole-Wrapped Single-Wall Carbon Nanotube. Journal of Physical Chemistry C, 2018, 122, 15979-15985.	3.1	7
25	Meyer–Neldel DC conduction in chalcogenide glasses. Pramana - Journal of Physics, 2011, 76, 629-637.	1.8	6
26	Vibrational density of states of TiO2 nanoparticles. Journal of Non-Crystalline Solids, 2013, 373-374, 28-33.	3.1	6
27	Solar Fuels: Tailoring Surface Frustrated Lewis Pairs of In <sub>2</sub> O <sub>3â^'</sub> <i><sub>x</sub></i> (OH) <sub>y</sub> for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO <sub>2</sub> by Isomorphous Substitution of In <sup>3+</sup> with Bi <sup>3+</sup> (Adv. Sci. 6/2018). Advanced Science, 2018, 5, 1870034	11.2	3
28	Photothermal Catalysis: Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO <sub>2</sub> with High Activity and Tailored Selectivity (Adv. Sci. 10/2017). Advanced Science, 2017, 4, .	11.2	2
29	Microstructural and Electronic Properties of the YSZ/CeO <sub>2</sub> Interface via Multiscale Modeling. Journal of Physical Chemistry C, 2020, 124, 15680-15687.	3.1	2
30	Disorder in energy materials and strategies to model it. Advances in Physics: X, 2021, 6, .	4.1	1
31	Structural properties of amorphous TiO2 nanoparticle: Molecular dynamics study. , 2011, , .		0
32	Static Structure Factor of Amorphous Rutile Nanoparticle: A Molecular Dynamics Study. , 2011, , .		0
33	Interfacial Properties of Bilayer SOFC Electrolytes Via Scale Bridging Simulations. ECS Meeting Abstracts, 2020, MA2020-01, 1801-1801.	0.0	Ο